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Fermionized Dipolar Bosons Trapped in a Harmonic Trap

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Abstract We explore entanglement properties of systems of identical dipolar bosons confined in a 1D harmonic trap by using explicitly correlated Jastrow-type wavefunctions. Results for the linear entropy in dependence on the dimensionless coupling and the number of particles are provided and discussed.

1 Introduction

The study of the properties of various systems of confined interacting particles is presently one of the most active areas of theoretical physics, which is due to the great technological development that has enabled the experimental realization of such systems. In particular, recent experimental progress has opened up perspectives for achieving systems with particles interacting through the dipole-dipole interaction (DDI) [1,2], which has inspired great interest in understanding their properties [3–6]. There has also been a growing interest in studying entanglement properties of quantum composite systems, since their entangled states are an essential ingredient for quantum computation. In particular, a number of papers have dealt with the entangled states of quantum systems composed of interacting particles, see for instance [7,8] and references therein. However, entanglement is systems with dipolar particles has not yet drawn much attention.

In this paper, we are going to shed some light on the entanglement properties of systems of particles confined in a harmonic trap

$$V(\mathbf{r}) = \frac{m}{2}(\omega^2 x^2 + \omega_\perp^2 \rho^2), \tag{1}$$

with the DDI modeled by

$$U(\mathbf{r}) = \frac{d^2}{|\mathbf{r}|^3}(1 - 3cos\theta_{rd}^2), \tag{2}$$

where θ_{rd} is the angle between $\mathbf{r}$ and $\mathbf{d}$, and d^2 is the strength of the DDI.

Here we restrict ourselves to the strictly 1D limit as $\lambda = \omega_\perp/\omega \to \infty$, in which the corresponding Hamiltonian takes the form [3,4]

$$H = -\frac{1}{2}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + V(x_1, x_2, \ldots, x_N) \tag{3}$$

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with

$$V(x_1, x_2, \ldots, x_N) = \sum_{i=1}^{N} \frac{1}{2} x_i^2 + \sum_{i<j} \frac{g}{|x_i - x_j|^3}. \tag{4}$$

The coordinates and the energies are measured in terms of $\sqrt{\hbar/m\omega}$ and $\hbar\omega$, respectively, and g is the dimensionless coupling: $g = -d^2\sqrt{\omega}m^{\frac{3}{2}}(1+3\cos 2\theta)/2\hbar^{\frac{5}{2}}$, where θ is the angle between $\mathbf{d}$ and the x axis. The coupling g is positive for $\theta_{crit} < \theta \leq \frac{\pi}{2}$, $\theta_{crit} = \arccos(1/\sqrt{3})$.

2 Results and Discussion

The system (3) of bosons gets fermionized for any $g \neq 0$. The ground-state bosonic wavefunction ψ_B is related via Bose–Fermi mapping to the lowest energy antisymmetric wavefunction ψ_F as $\psi_B = |\psi_F|$ [9]. In particular, in the limit as $g \to 0$, we have

$$\psi_B^{g\to 0}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} |\det_{n=0,j=1}^{N-1,N}(\varphi_n(x_j))|, \tag{5}$$

where φ_n are the eigenfunctions of the 1D harmonic oscillator with frequency $\omega = 1$, which means that the system (3) forms a Tonks–Girardeau gas as $g \to 0$. On the other hand, in the strong interaction limit as $g \to \infty$, where the harmonic approximation (HA) is valid, the ground-state bosonic wavefunction takes the form [7,8]

$$\Psi_B^{g\to\infty}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \sum_p \psi(x_{p(1)} - x_1^c, x_{p(2)} - x_2^c, \ldots, x_{p(N)} - x_N^c), \tag{6}$$

with

$$\psi(z_1, z_2, \ldots, z_N) = \prod_{i=1}^{N} \left(\frac{\omega_i}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\omega_i \zeta_i^2(z_1, z_2, \ldots, z_N)}{2}}, \tag{7}$$

where the sum goes over all permutations, ω_i^2 are the eigenvalues of the Hessian matrix $[\partial_{x_m}\partial_{x_n} V|_{\{x_1^c,\ldots,x_N^c\}}]_{N\times N}$, $\{x_i^c\}$ are the classical equilibrium positions of the particles, and $\{\zeta_i\}$ are the corresponding normal modes. We recall that in the limit as $g \to \infty$ a perfect Wigner crystal state is formed, i.e., the particles localize themselves around their classical equilibrium positions and their clouds do not overlap.

For finding the bosonic ground-state approximate wavefunction of (3) for finite values of g, we apply a simple trial wave function given by a Jastrow-type wavefunction [10]:

$$\chi(x_1, x_2, \ldots, x_N) \propto \prod_{k=1}^{N} e^{-\frac{x_k^2}{2}} \prod_{i>j}^{N} f\left(\alpha \frac{x_i - x_j}{\sqrt{2}}\right), \tag{8}$$

with

$$f(x) = e^{\frac{x^2}{2}} \phi(x), \tag{9}$$

where ϕ is the ground-state relative motion wavefunction of the corresponding two-particle system, namely

$$H^x = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{g}{2^{\frac{3}{2}}|x|^3}, \tag{10}$$

and α is a variational parameter that is optimized in order to minimize the expectation value of the energy. It was recently shown that the ansatz (9) is an effective tool for estimating both the energy [10] and the entanglement characteristics [8] of 1D systems with a harmonic trap. In order to solve the eigenproblem with (10), we apply the Rayleigh–Ritz (RR) method, which uses, as a variational trial function, a linear combination of a finite set from the pseudoharmonic oscillator basis

$$v_n(x) \sim |x|^{\beta - \frac{1}{2}} e^{-\frac{1}{2}x^2} {}_1\mathrm{F}_1(-n; \beta; x^2), \tag{11}$$

$u_n(0) = 0$, where $\beta > \frac{3}{2}$ and ${}_1\mathrm{F}_1$ is the Kummer's confluent hypergeometric function. In the present calculations, we use a 20-term RR wavefunction. For more details on this point, see [11].

The key quantities for determining the quantum-mechanical properties of N- particle systems is the one-particle reduced density matrix (RDM)

$$\rho(x, y) = \int_{\Re^{N-1}} \Psi(x, x_2, \ldots, x_N)\Psi(y, x_2, \ldots, x_N) \prod_{k=2}^{N} dx_k, \tag{12}$$

From the quantum information point of view, its diagonal representation characterizes the entanglement in the system. Here we will measure the amount of the entanglement via the linear entropy of the one-particle RDM

$$\begin{aligned} L &= 1 - \int_{\Re^2} [\rho(x, y)]^2 dxdy \\ &= 1 - \int_{\Re^{2N}} \Psi(x, x_2, \ldots, x_N)\Psi(y, x_2, \ldots, x_N)\Psi(x, x_2', \ldots, x_N')\Psi(y, x_2', \ldots, x_N') \prod_{k=2}^{N} dx_k dx_k' dxdy. \end{aligned} \tag{13}$$

For the ground-state of the systems under consideration, the linear entropy can be easily obtained in two limiting situations discussed in the previous subsection, namely the cases $g \to 0$ and $g \to \infty$. In the first case, this can be done with the use of an algorithm presented in [12], and in the second, by applying the HA [7,8]. For finite values of g, we perform the integration in Eq. (13) numerically.

Figure 1 depicts our numerical results for the dependencies of the linear entropy L_g^N on g and N, where the horizontal lines mark the results obtained within the framework of the HA in the limit $g \to \infty$. It is worth mentioning that the linear entropy exhibits a discontinuity at the point $g = 0$, regardless of N. Namely, it tends to a finite value as $g \to 0$, determined by (5), while at $g = 0$, where the wavefunction is the product function $\Psi_B^{g=0} = \prod_{i=1}^{N} \varphi_0(x_i)$, it has the value 0, reflecting the fact that entanglement is absent. As may be seen from Fig. 1, in each case considered, the linear entropy converges with an increase in g, to its asymptotic value predicted by the HA in the $g \to \infty$ limit, which confirms both the correctness of our calculations and the effectiveness of the ansatz (9). We recall that the perfect Wigner crystal state corresponds to the situation in which the localized wave packets of the particles do not overlap at all, which exactly takes place solely as $g \to \infty$. There may be a general interest in noting that an increase in the amount of entanglement resulting from an increase in N is almost insensitive to changes in g. Such a behavior of the entanglement is clear in the Wigner crystallization regime, but it is a bit surprising in the range of small values of g in which the entanglement is substantially sensitive to changes in g. We have verified that the following approximation holds well: $L_g^N \approx L_2^N + L_{g\to\infty}^N - L_{g\to\infty}^2$, which gives $\partial_g L_g^N \approx \partial_g L_2^N$. It can be expected that this approximation also holds well for larger systems than those considered here. It is worth noting that the change in the value of the linear entropy produced by the addition of one particle to the N-particle system is smaller, the larger is N.

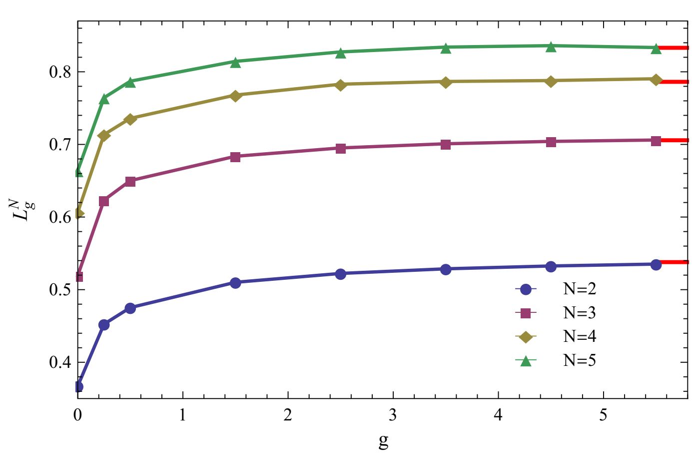

Fig. 1 The dependence of the linear entropy of the bosonic ground-state on g for $N = 2, \ldots, 5$

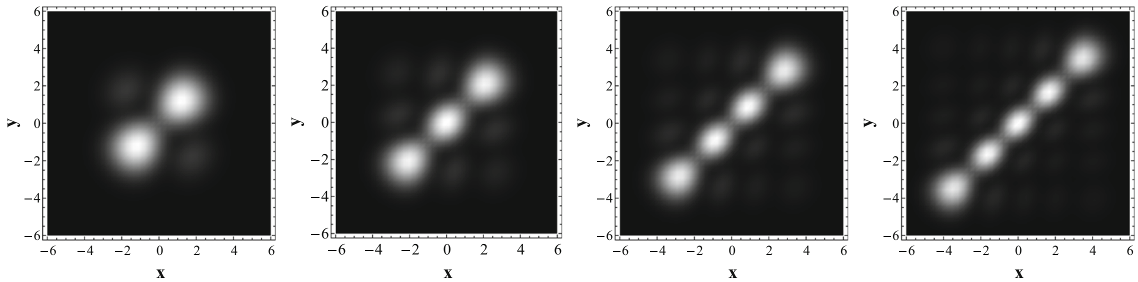

Fig. 2 Plots of the RDM for $N = 2, \ldots, 5$ at $g = 5.5$

The entanglement makes thus its most rapid variation in the range of small values of N. One can expect from the results of Fig. 1 that at least in all cases considered here the value of g at which the transition to the Winger crystal phase occurs hardly depends on the number of particles. Plots of the corresponding $\rho(x, y)$ shown in Fig. 2 clearly confirm this guess.

3 Summary

We studied the strictly 1D systems of dipolar particles confined in a harmonic trap with the use of the Jastrow-type wavefunctions constructed from the relative motion wavefunction computed with the use of the spiked oscillator basis, which is effective for such systems. Our results showed the effects of the dimensionless coupling g and the number of particles N on the entanglement. Both the sensitivity of the linear entropy to changes in g and the point g at which a transition to the Wigner molecule state occurs are almost independent of N. The most rapid variation of the entanglement takes place in the ranges of small values of g and N.

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